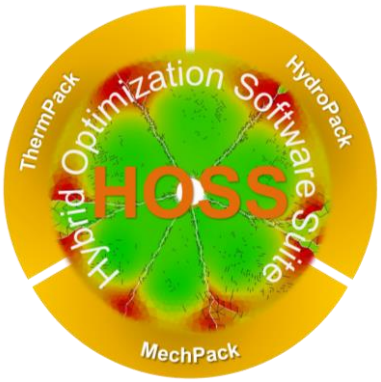
Los Alamos National Laboratory
Request for Proposal
Hybrid Optimization Software Suite (HOSS) - Commercialization Opportunity

Los Alamos National Security, LLC ("LANS") is the manager and operator of the Los Alamos National Laboratory ("LANL") for the U.S. Department of Energy's ("DOE's") National Nuclear Security Administration under contract DE-AC52-06NA25396. LANS is a mission-centric Federally Funded Research and Development Center focused on solving the most critical national security challenges through science and engineering for both government and industry sectors. LANS is currently seeking an industry partner(s) to assist with the commercial deployment of its *Hybrid Optimization Software Suite (HOSS)* technology portfolio.

BACKGROUND AND TECHNOLOGY DESCRIPTION

HOSS was born from a desire for LANL to create a numerical tool that could simulate extreme high strain rate events in harsh subsurface environments, i.e., underground nuclear explosions. The ideal tool would have to be able to handle: high strain rate events, fracture and fragmentation, a diverse suite of material models (plasticity, anisotropy, stochasticity, etc.), in-situ stress pre-conditioning and in-situ geologic structures (fracture networks, faults, joints, etc.). Over the past decade LANL researchers (along with collaborator and computational mechanics authority Dr. Antonio Munjiza of Tetcognition Limited) have developed such a tool (HOSS), which is based on the Combined Finite-Discrete Element Methodology (FDEM).



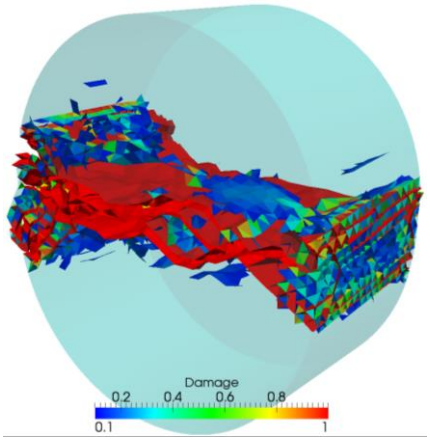
HOSS is used to describe material deformation and failure (i.e., fracture and fragmentation) under a number of user-prescribed boundary conditions. Some of the key general features of HOSS are:

- Finite element formulation allowing for finite strain deformation and finite displacements;
- Damage formulation with explicit handling of fracture and fragmentation processes;
- Resolution of contact dynamics among a large number of interacting particles;
- 2D/3D and 2.5D (shell) finite elements designed to avoid shear- and volumetric-locking problems;
- Handling of 2D/3D and 2.5D general irregular-shaped particles (discrete elements);
- Material model formulation designed to handle either isotropic or anisotropic materials (fields of application: non-homogenous/bedded rocks, laminated materials, composite materials, wood, biological materials, etc.);
- Interaction formulation for handling rock joints;
- Integrated solid-fluid solver (ISF) designed for fluid-driven material deformation such as hydrofracture and related processes;

- Explicit modeling of fluid flow through fractures, flow through porous reservoirs and flow between fractures and porous matrix including processes such as caking in oil extraction;
- Material models to handle evolution of porosity;
- Fully parallel in 2D/3D and 2.5D; and
- Supports multi-stage simulations.

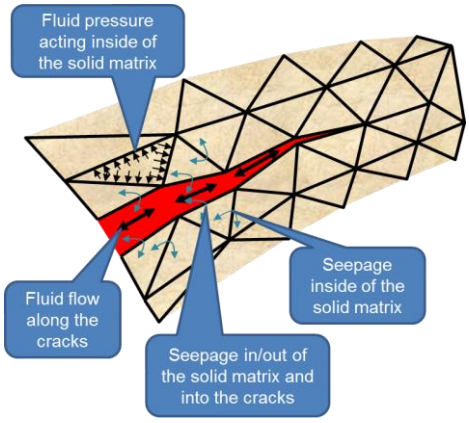
HOSS is composed of three general purpose software suites called MechPack, HydroPack and ThermPack. Designed with modularity in mind, the code can be easily extended to accommodate a variety of other physics suites such as chemical processes.

- **MechPack**: This suite serves as the core of HOSS. It contains state-of-the-art algorithms not currently available in any other current commercial or research package. Functional elements of MechPack include:
    - Hybrid (continuum-discontinuum) formulation:
        - The latest combined smeared and discrete crack, fracture and fragmentation models; and
        - The solver is able to efficiently handle simulations on a wide range of length scales, from micro- to large-scale (hundreds of meters).



    - Continuum formulation:
        - Unified hypo-hyper approach with multiplicative decomposition-based large strain deformability in 2D/3D and 2.5D;
        - Selective integration-based finite element (FE) library for a whole family of finite elements, i.e., from solids to shells and membranes. This library can be extended on demand (new finite element formulations can be developed on request within the code);
        - Linkage to nonlinear material packages thus enabling the incorporation of finite strain based material nonlinearity;
        - Anisotropic properties of the solid can be specified on a FE by FE basis; and
        - Formulation designed to avoid FE volumetric- and shear-locking problems.
    - Discontinuum formulation:
        - State of the art contact detection algorithms that are highly efficient for 2D/3D and 2.5D general shape particles; and
        - Latest generation contact force algorithms for 2D/3D and 2.5D.
    - Material modeling:
        - A unified constitutive approach featuring a generalized nonlinear anisotropic non-homogeneous (isotropic naturally included) large strain material description. This enables the code to simulate materials such as layered rocks, laminates, composites, wood, biological materials, etc.;
        - Interfaces created within the software to allow handling of other types of material models, or user added material models;
        - Incorporates stochastic framework for seeding of input parameters (joint properties, elastic properties, fracture properties, etc.); and
        - Explicit handling of in-situ rock joints.
- **HydroPack**: This suite is based on an ISF designed to capture the effects of fluids, gas, and saturation within a porous medium. It is ideal for the simulation of hydrofracking operations,

liquefaction effects, CO_2 sequestration and utilization, blasting, geo-thermal energy extraction, slope stability analysis and similar field problems (*See* the patent application referenced in the "LANS HOSS Intellectual Property Portfolio" section). HydroPack features include:



  - Explicit description of:
    - Transient and steady state flow through crack manifolds;
    - Transient and steady state flow through existing rock joint manifolds;
    - Transient and steady state anisotropic flow through porous geo-material (seepage); and
    - Multi regime fluid solver (subsonic, supersonic).
  - Integration of solid and fluid phases at material point level. This results in effective stress description for the solid, i.e., fluid-driving-solid and solid-compressing-fluid (fluid pressure inside the porous rock matrix).
- **ThermPack**:
  This suite complements both the MechPack and the HydroPack. ThermPack features are:
  - Heat transfer within the solid portion of the domain;
  - Liquid medium heat transport through the porous solid and cracks;
  - Reacting fluid flow such as (but not limited to) burning propellant;
  - Non compressible flow taking into account both, energy transport and energy sources (reactions); and
  - Heat effects on solid material properties (softening, melting, etc.).

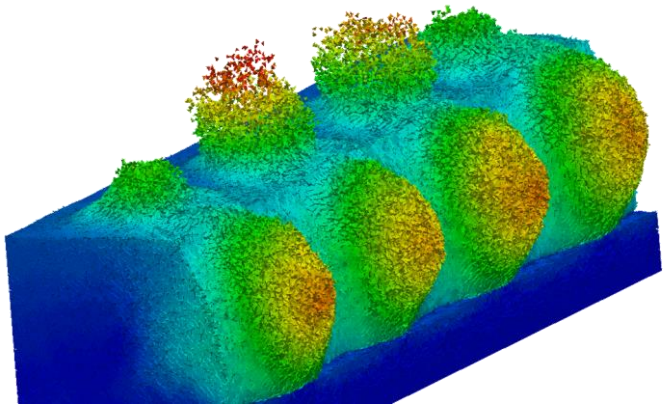
Other differentiating elements of the HOSS tool include:

- **Parallelization**:
  - HOSS uses specially designed parallelization engines tailored for easy portability to different hardware platforms ranging from desktops to 10,000+ node clusters;
  - Grand scale parallelization in 2D and 3D achieving efficiency of over 90% on high performance computer clusters (1,000+ nodes); and
  - Tailor-made data compression, data gathering and data handling solutions.
- **Multi-Stage Simulations**:
  - Functionality needed to model complex systems including user pre-defined in-situ stress distribution, pumping stages for hydrofracking simulations, etc.;
  - Modification of boundary conditions and solvers for each restart supported; and
  - Incorporates object-oriented binary data structure.
- **Pre-processing:**
  - XML–based input files in ASCII and binary formats, which can be combined together;
  - Robust ASCII–based input file reader designed to be user-friendly; and
  - Provides mesh translator for major model meshing formats and extension of mesh translator to user-preferred meshing formats.
- **Post-processing:**
  - Accommodates commonly-used post-processing formats (e.g., VTK, GMV, etc.);
  - Novel post processing tool (MVIS) tailor-made for grand scale visualization – optimized for visualizing systems with more than 100 million particles on a PC;
  - Specially designed data compression algorithm for output of grand scale simulation results; and

- Supports output of related historical data.

HOSS features state-of-the-art FDEM algorithms which have been extensively proven in rock mechanics and other fields. The breadth of applications for HOSS is wide and includes, but is not limited to the following areas:

- Experimental rock mechanics (triaxial, uniaxial, etc.)
- Hydrofracture (Oil and Gas, CO_2 sequestration and utilization, geothermal energy)
- Wellbore integrity and drilling (Oil and Gas, CO_2 sequestration and utilization, geothermal energy)
- Slope stability (Mining, road infrastructure design)
- Block caving (Mining)
- Excavation damaged zone for underground operations (Mining, Waste storage, natural resources storage)
- Pillar stability (Mining)
- Analysis of reinforcement/modifications to historical monuments and buildings
- Dam stability analysis
- Subsurface stress & induced seismicity
- High velocity impact studies
- National security
- Architectural glass
- Nano mechanics
- Materials by design
- Bone fracture modeling
- Red blood cell flow modeling
- Membranes



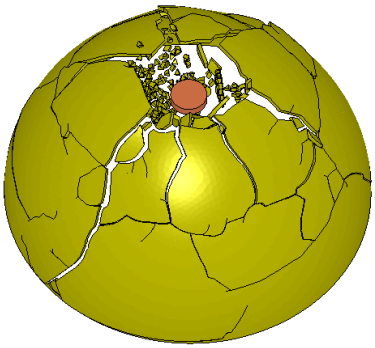
The extensive technology development efforts undertaken by the Los Alamos HOSS research and development team have resulted in a technology readiness level of 6 ("TRL 6"). To achieve broad commercial deployment of the HOSS technology, LANS is actively seeking one or more commercial partners to further collaborate and further develop these technologies for market applications. In particular, LANS is exploring multiple mechanisms to ensure the vitality of its internal research and development program for government customers while accelerating the broader adoption and deployment of this technology for commercial applications with private sector partners.

POTENTIAL AREAS FOR PARTNERSHIP

The Los Alamos team has identified several areas for partnership and/or commercial licensing to advance the LANS HOSS technology. LANL has already begun work on some of these topics and collaboration with a commercialization partner could accelerate the added functionality that includes:

- Future implementation of rock joints to include a 3D handling capability;
- Extension of the ISF from single phase to multi-phase capability;
- ThermPack development;

- Further integration of time scales that will extend to scales ranging from milliseconds to days, months or years via the incorporation of a pseudo-implicit time integration approach;
- Future implementation of finite element handling to include membrane elements as well as 2D and 3D beam and rod element handling;
- Implementation of explosive burn modeling: deflagration and detonation;
- Development of non-reflecting and periodic boundaries; and
- Software engineering and GUI development for pre- and post-processing.



The foregoing list is non-exhaustive and LANS is open to evaluating commercial interest in other applications and areas for collaboration that are not identified above. LANS is opening this formal Request for Proposal to commercial entities to identify potential collaboration partners and/or licensees to achieve commercial deployment of the LANS HOSS technology. This offering is made without prejudice to any form of agreement, collaborative arrangement, alliance, number of entities, or partnering mechanism. ***Those companies interested in pursuing this commercialization opportunity should direct a letter or response, as well as any comments or questions, to the undersigned on or before Wednesday, March 9, 2016.***

Below you will find the following: 1) a listing of the relevant LANS Intellectual Property; 2) details regarding the information requested in the form of a Commercialization Proposal; and 3) information regarding the next steps in the commercialization call process.

LANS HOSS INTELLECTUAL PROPERTY PORTFOLIO

Patent Applications:
S133043 entitled "Integrated Solver for Fluid Driven Fracture and Fragmentation," U.S. nonprovisional patent application number 14/339,760 filed July 24, 2014, first filing date July 26, 2013.

Copyrights:
International copyright on HOSS software.

Please note that the U.S. Government retains a worldwide, royalty-free, non-exclusive right to practice any LANS-owned patents and/or copyrighted software.

PREFERRED PARTNER ATTRIBUTES

The following is a list of the preferred partner attributes:

- Demonstrated knowledge of product marketing, sales, and worldwide software distribution;
- Ability to set up software licensing and security mechanisms (or equivalent) for appropriate protection of source and executable versions of the code;
- Software marketing and packaging expertise to perform the following:
  - Make a beta version of the software available for testing;
  - Make an educational version of HOSS available at no/low cost to graduate research students to promote the adoption of HOSS;
- Ability to provide or acquire support for maintenance and further development of the HOSS suite; and

- Expertise to continue development of the tool to enhance its functionality around the technical areas listed in the "Potential Areas for Partnership" section
- Partner willingness to engage in continued R&D around the technology related to potential new developments of HOSS

Commercialization Proposal

LANS will select the most qualified collaboration partner(s) / licensee(s) based on a review and analysis of all Commercialization Proposals submitted for consideration.

Your Commercialization Proposal should include the following information:

- Description of your company and its mission;
- Explanation of your company's interest in the technology and its relevance to the company's goals and product offering(s);
- Explanation of the scope of rights your company would need in a license from LANS to fully leverage the HOSS technology to meet your goals and objectives;
- Articulation of your company's business strategy for deploying HOSS for various applications (e.g., goal for releasing HOSS via cloud deployment or other avenue identified by your company; etc.);
- Proposal for how your company would address adding the proposed functional elements identified in the "Potential Areas for Collaboration" for each of the components to the extent your company is interested in working with LANL to enhance the tool with those added elements;
- Identification of any additional functional elements not identified in "Potential Areas for Collaboration" your company may have interest in exploring;
- Marketing strategy to identify ideal points of market entry for the HOSS tool;
- Demonstrated experience in developing and marketing a technology in one or more of these application areas identified for HOSS;
- Brief description of your company's financial and human resources available for commercializing this technology; and
- Any questions that you would like to have answered during a follow-on discussions related to HOSS commercialization.

WHAT WE ARE REQUESTING

If you are interested in exploring this commercialization opportunity, please submit the required Commercialization Proposal on or before ***Wednesday, March 9, 2016.*** Your Commercialization Proposal should include, at a minimum, the items listed above; however, you are welcome to include any additional information regarding your company (brochures, product information, etc.) that may help us to evaluate your interest and suitability as a commercialization partner. Depending upon the responses that we receive, LANS may host a follow-on Webinar and/or Commercialization Workshop to provide additional details regarding this commercialization opportunity. ***Note: please properly mark any information that your company considers proprietary or business-sensitive. LANS will supply a Non-Disclosure Agreement (NDA) to companies that require such protection. NDAs with Non-U.S. companies will require additional time to process due to export control requirements.***

We look forward to reviewing your ideas on how together we can rapidly advance this technology towards the commercial marketplace and accelerate deployment to the benefit of the U.S. economy. Please respond by email to Kathleen_m@lanl.gov, or call Kathleen McDonald at 505/667-5844. You can also contact Don Hickmott. Don can be reached via email at dhickmott@lanl.gov or by phone at 505/667-8753. In order for your Commercialization Proposal to be considered responsive, it must be received by ***COB on Wednesday, March 9, 2016.***. Proposals may be sent to the contact listed below or submitted via email.

LANL Business Development Contacts – Richard P. Feynman Center for Innovation:

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